

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
 Data File : BF102164.D
 Acq On : 17 Jan 2018 21:41
 Operator : SJ/JU
 Sample : J1167-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72-11995

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	477	482	489	rVB	167900	223786	8.43%	0.981%
2	5.328	546	551	555	rBV	2467125	2576161	97.09%	11.291%
3	6.357	721	726	730	rBV	2578519	2592751	97.72%	11.364%
4	6.486	744	748	751	rBV	2756336	2653347	100.00%	11.629%
5	6.722	784	788	791	rBV	976211	815351	30.73%	3.574%
6	6.875	810	814	817	rBV	2410401	2004148	75.53%	8.784%
7	7.286	879	884	887	rBV	1730009	1585504	59.75%	6.949%
8	7.998	1001	1005	1009	rBV	1145508	1034852	39.00%	4.536%
9	8.557	1096	1100	1104	rBV	156430	132649	5.00%	0.581%
10	9.080	1184	1189	1192	rBV	2921453	2522135	95.05%	11.054%
11	9.474	1252	1256	1259	rBV	308771	271865	10.25%	1.192%
12	9.751	1299	1303	1307	rBV	1022234	964211	36.34%	4.226%
13	10.469	1421	1425	1428	rBV	439793	373336	14.07%	1.636%
14	10.539	1433	1437	1440	rBV	1400762	1176122	44.33%	5.155%
15	11.233	1551	1555	1559	rBV	876221	705949	26.61%	3.094%
16	12.815	1820	1824	1828	rBV	1606530	1472045	55.48%	6.452%
17	13.709	1973	1976	1985	rBV	165949	179625	6.77%	0.787%
18	13.862	1998	2002	2006	rBV	686338	671717	25.32%	2.944%
19	14.345	2078	2084	2092	rBV9	24893	54847	2.07%	0.240%
20	14.498	2107	2110	2114	rBV4	23272	28873	1.09%	0.127%
21	15.280	2238	2243	2247	rBV	614695	716204	26.99%	3.139%
22	15.768	2322	2326	2334	rBV7	32806	60701	2.29%	0.266%

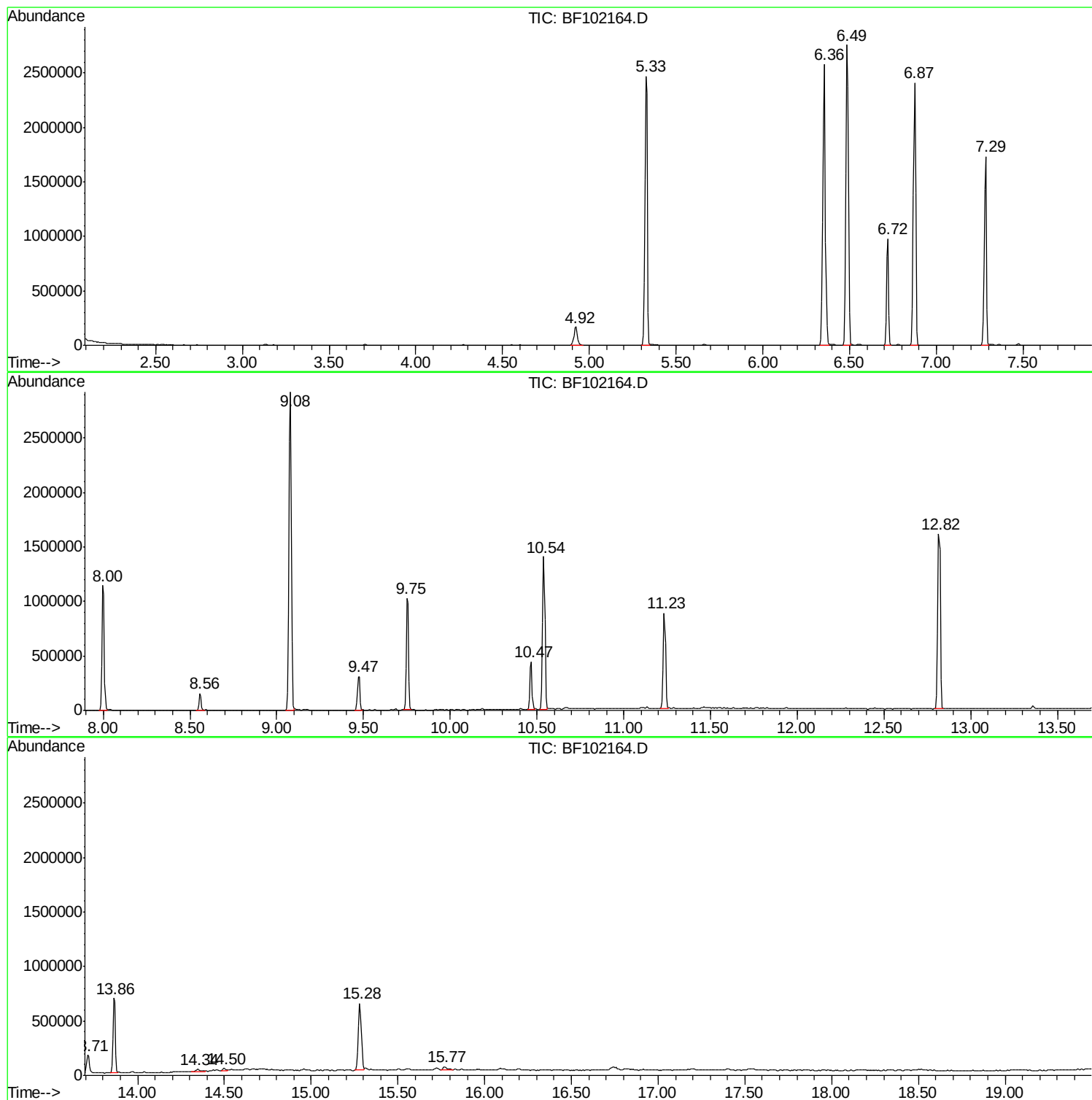
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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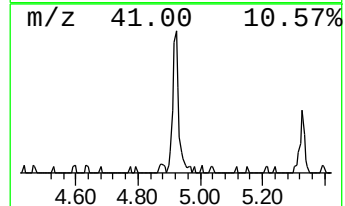
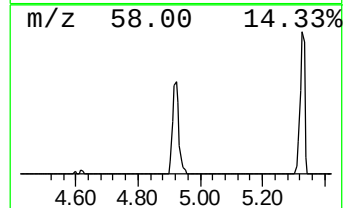
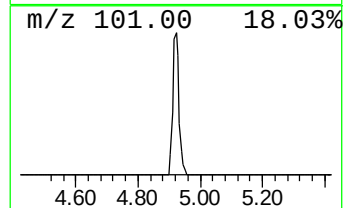
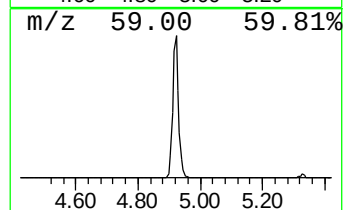
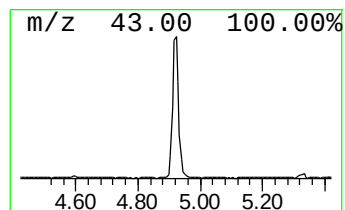
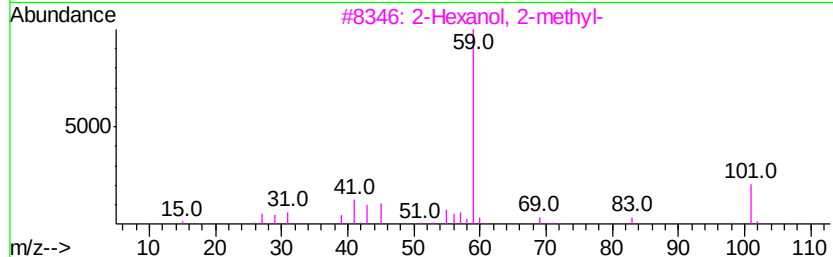
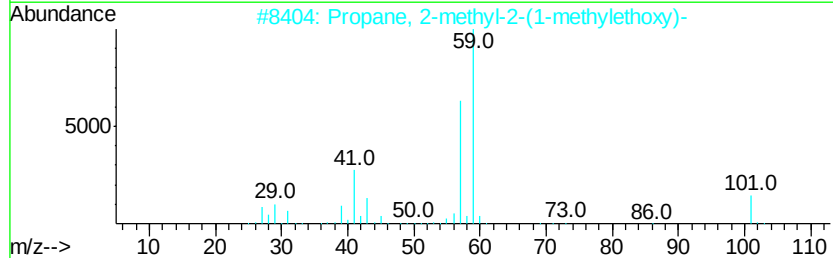
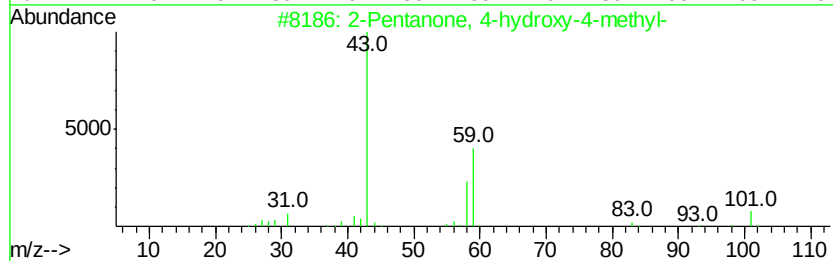
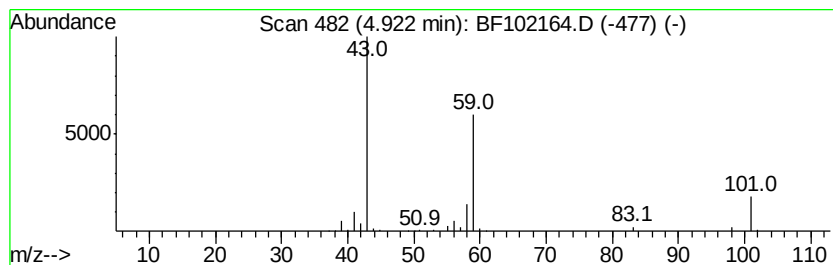
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.49 ng	223786	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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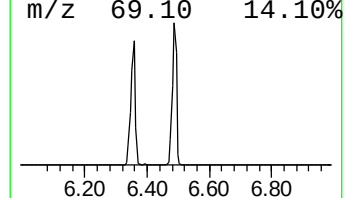
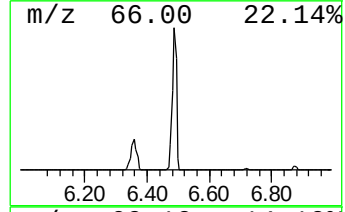
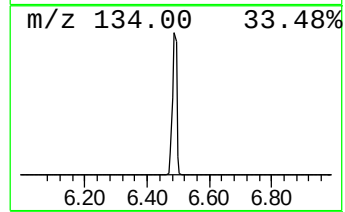
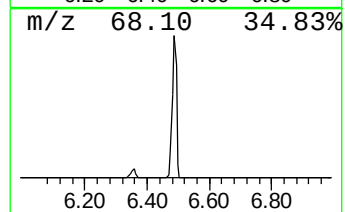
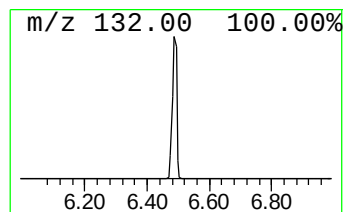
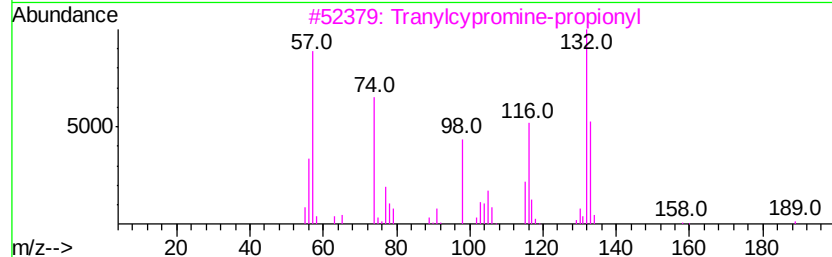
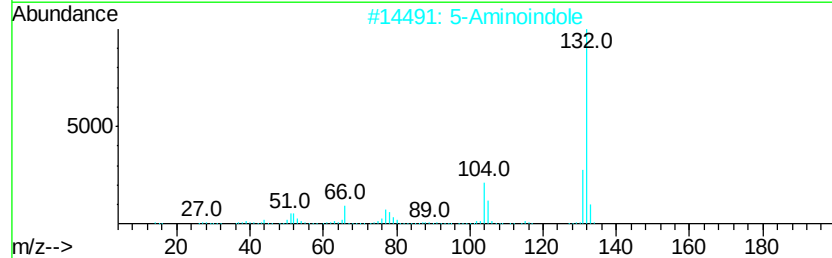
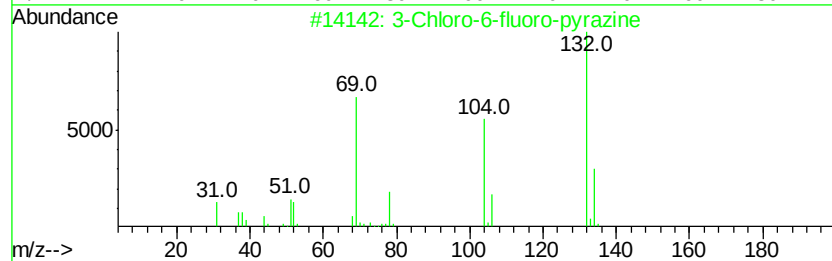
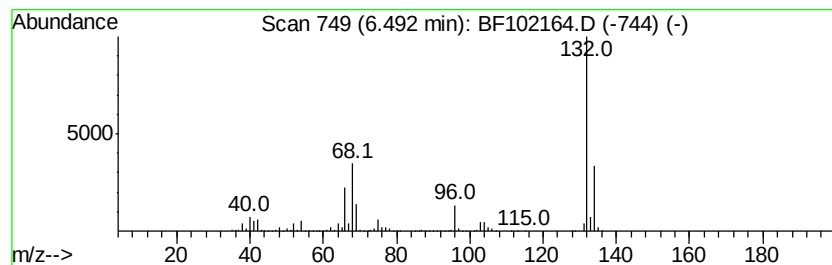
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	65.08 ng	2653350	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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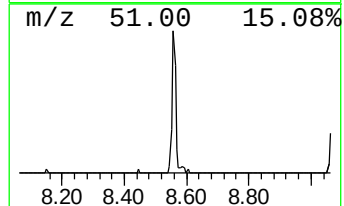
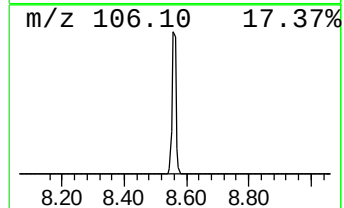
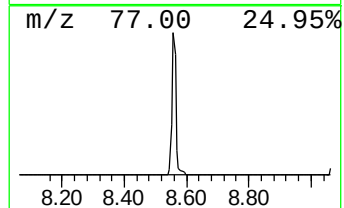
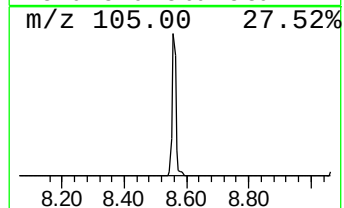
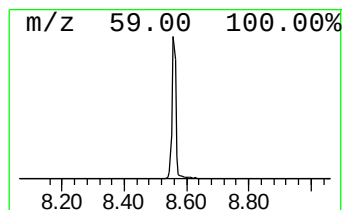
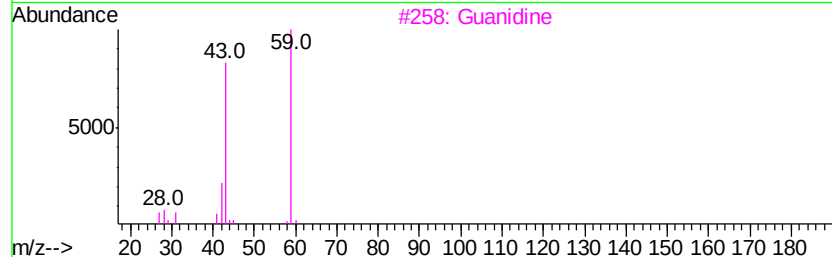
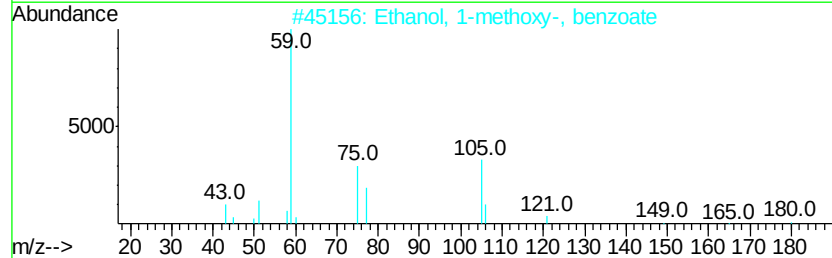
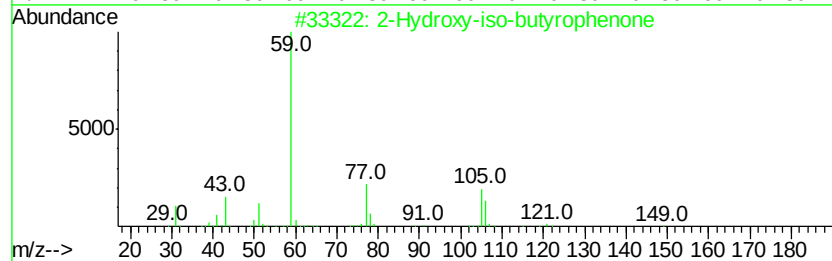
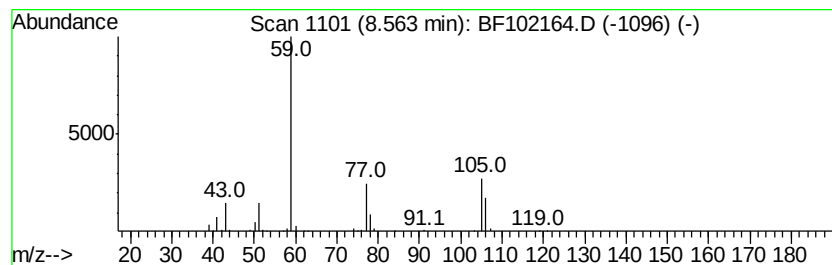
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	2.56 ng	132649	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3		Guanidine	59	CH5N3	000113-00-8	9
4		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9



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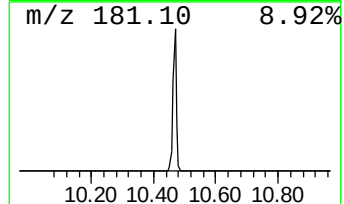
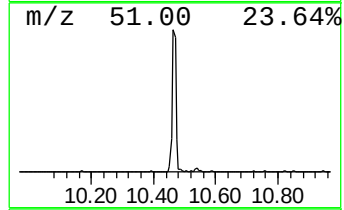
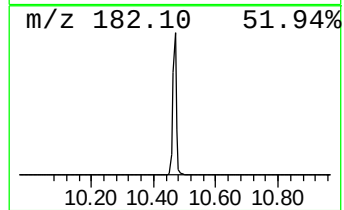
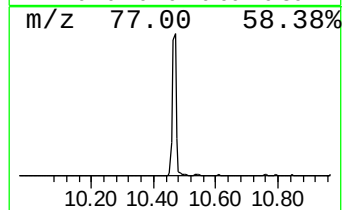
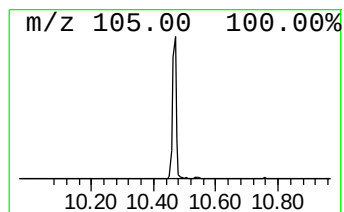
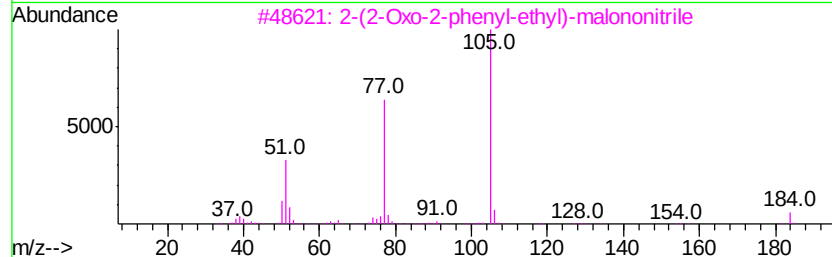
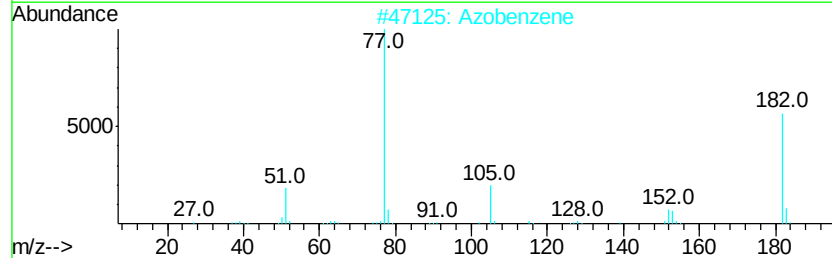
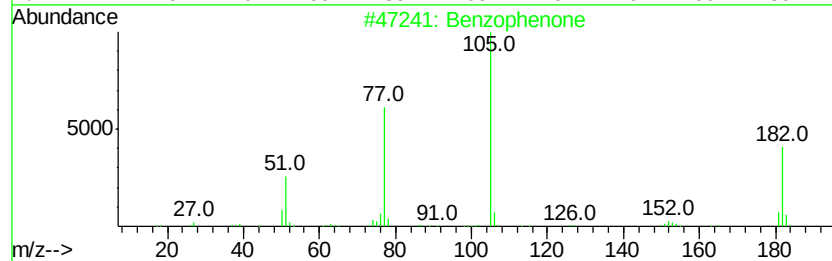
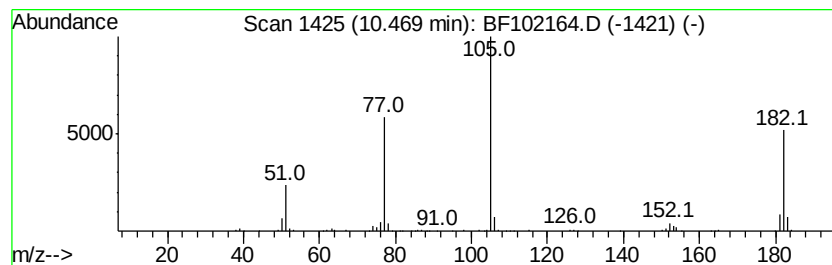
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.47	7.74 ng	373336	Acenaphthene-d10		9.75	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Azobenzene	182	C12H10N2	000103-33-3	64
3		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4		Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5		N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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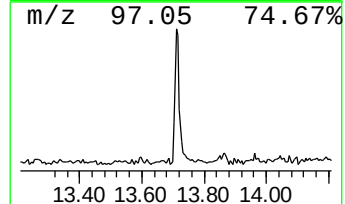
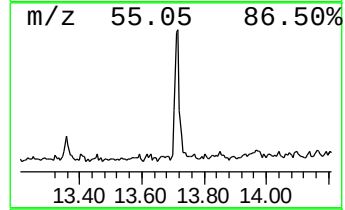
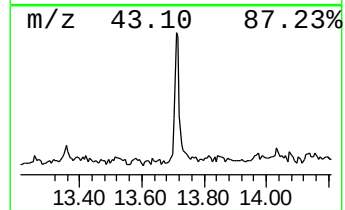
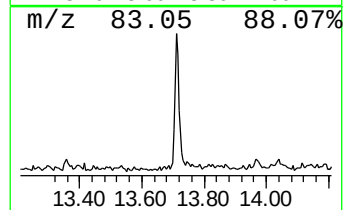
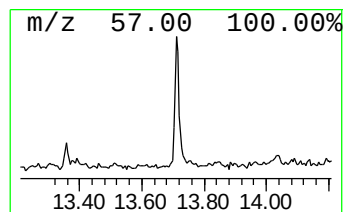
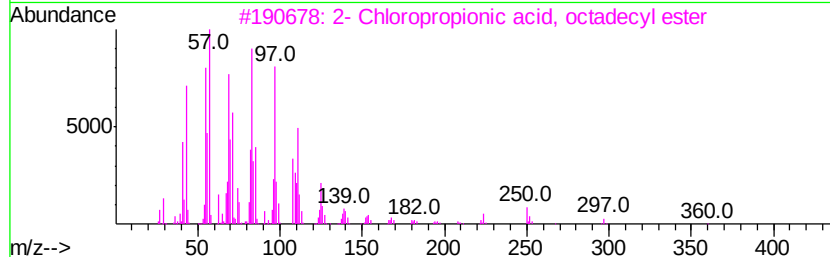
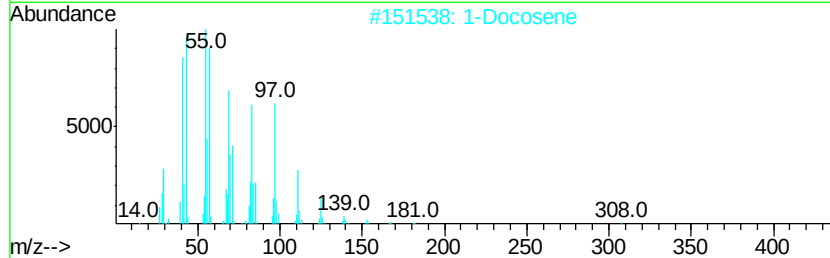
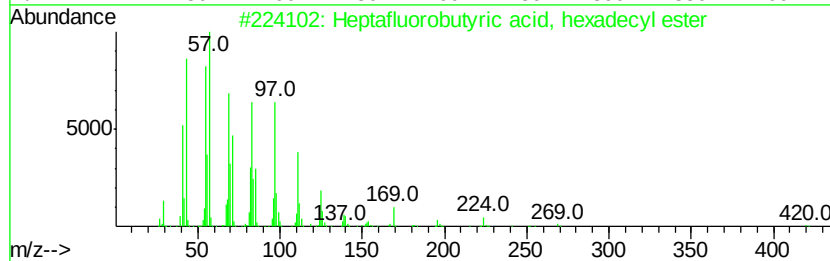
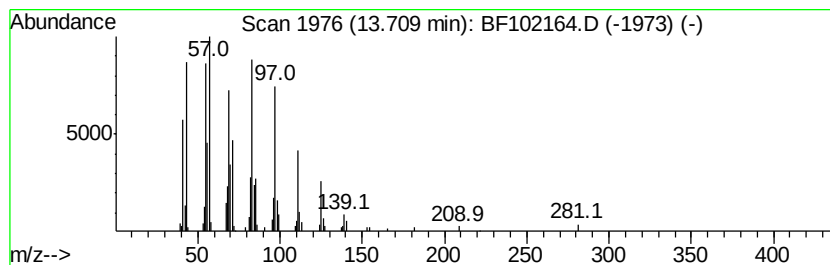
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Peak Number 6 Heptafluorobutyric acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.35 ng	179625	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
2	1-Docosene	308	C22H44	001599-67-3	91
3	2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	5.5	ng	223786	1	6.72	815351	20.0
unknown6.49	6.49	65.1	ng	2653350	1	6.72	815351	20.0
2-Hydroxy-iso-but...	8.56	2.6	ng	132649	2	8.00	1034850	20.0
Benzophenone	10.47	7.7	ng	373336	3	9.75	964211	20.0
Heptafluorobutyri...	13.71	5.3	ng	179625	5	13.86	671717	20.0